# Momentum conservation implies anomalous energy transport in 1d classical lattices

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Under very general conditions, we prove that for classical many-body lattice Hamiltonians in one dimension (1D) total momentum conservation implies anomalous conductivity in the sense of the divergence of the the Kubo expression for the coefficient of thermal conductivity, $\kappa$. Our results provide rigorous confirmation and explanation of many of the existing "surprising" numerical studies of anomalous conductivity in 1D classical lattices, including the celebrated Fermi-Pasta-Ulam problem.

Since the pioneering work of Fermi, Pasta, and Ulam (FPU) revealed the "remarkable little discovery" [1] that even in a strongly nonlinear one-dimensional (1D) classical lattices recurrences of the initial state prevented the equipartition of energy and consequent thermalization, the related issues of thermalization, transport, and heat conduction in 1D lattices have been sources of continuing interest (and frustration!) for several generations of physicists. The complex of questions following from the FPU study involves the interrelations among equipartition of energy (is there equipartition ? in which modes ?), local thermal equilibrium (does the system reach a well-defined temperature locally ? if so, what is it ?), and transport of energy/heat (does the system obey Fourier's heat law ? If not, what is the nature of the abnormal transport ?) In sorting through these questions, it is important to recall that the study of heat conduction (Fourier's heat law) is the search for a non-equilibrium steady state in which heat flows across the system, but the situation is usually analyzed, using the Green-Kubo formalism of linear response [2], in terms of the correlation functions in the thermal equilibrium (grand canonical) state. A series of reviews spread over nearly two decades has provided snapshots of the understanding (and confusion) at different stages of this odyssey [3, 4, 5, 6, 7, 8].

Much of the past effort has been devoted to attempts to verify Fourier's law of heat conduction

$$\langle \vec{J} \rangle = \kappa \nabla T, \tag{1}$$

where in 1D the gradient is replaced by the derivative with respect to $x$. Here, $\kappa$ is the transport coefficient of thermal conductivity. Strictly speaking, $\kappa$ is well defined only for a system that obeys Fourier's law and where a *linear* temperature gradient is established (for small energy gradients such that relative temperature variation across the chain is small; in general $\kappa$ is a function of temperature, of course). In the literature the dependence of $\kappa(L)$ on the length $L$ of the chain has also been used to characterize the (degree of) anomalous transport. However, the definition of $\kappa$ for an anomalous conductor, where no internal temperature gradient may be established, is ambiguous. Typically, one defines it in the "global" sense, as $\kappa(L) \equiv \kappa_G \equiv JL/\Delta T$, where $\Delta T$ is the total temperature difference between the two thermal baths. However, if the temperature gradient is *not* constant across the system, one can define a local $\kappa$, $\kappa \equiv \kappa_L \equiv \frac{J}{\nabla T}$, where $\nabla T$ is the local thermal gradient. In the present article, we will distinguish between these two definitions and point out the places where failing to make this distinction has caused confusion in the literature. A very wide range of results have been produced by previous studies of different systems:

- in acoustic harmonic chains, rigorous results [9], establish that no thermal gradient can be formed in the system, with the result that formally $\kappa_G \sim L^1$, which can be understood heuristically by stability of the linear Fourier modes and the absence of mode-mode coupling;

- in the "Toda lattice," an integrable lattice model [10, 3], in which the result $\kappa_G \sim L^1$ can be understood in terms of stable, uncoupled *nonlinear* modes, the solitons, which are a consequence of the system's complete integrability [7];

- in non-integrable models with smooth potentials, including (i) the FPU system, leading eventually to claim that chaos was necessary and sufficient for normal conductivity ($\kappa_G = \kappa_L \sim L^0$) [8], a claim that has been countered by convincing numerical evidence for anomalous conductivity in FPU chains ( $\kappa_L \sim L^{0.4}$ ) [11, 12]; (ii) the diatomic (and hence non-integrable) Toda lattice, where initial numerical results claiming $\kappa_L \sim L^0$ [13] have recently been refuted by a more systematic study showing $\kappa_L \sim L^{0.4}$ [14]; and(iii) the "Frenkel-Kontorova model," where recent studies have shown that (at least for low temperatures) $\kappa_L \sim L^0$ [15];

- in non-integrable models with hard-core potentials, including (i) the "ding-a-ling" model [16]; and (ii) the "ding-dong" model [17], both showing convincingly that $\kappa_L = \kappa_G \sim L^0$.

This bewildering array of results has recently been partially clarified in a series of independent but overlapping studies. The numerical studies of Hu *et al.* [15] and of Hatano [14] show that *overall momentum conservation* appears to a key factor in anomalous transport in 1D lattices. Lepri *et al.* [18, 19] and Hatano[14] have argued that the anomalous transport in momentum conserving systems can be understood in terms of low frequency, long-wavelength "hydrodynamic modes" that exist in typical momentum-conserving systems and that hydrodynamic arguments may explain the exponents observed in FPU [18, 19] and diatomic Toda lattice [14].

In the present work, we extend and formalize these recent results and resolve finally at least one important aspect of conductivity in 1D lattices: namely, we present a rigorous proof that in 1D conservation of total momentum implies anomalous conductivity.

We consider the general class of classical one-dimensional many-body Hamiltonians

$$H = \sum_{n=0}^{N-1} \left( \frac{1}{2m_n} p_n^2 + V_{n+1/2}(q_{n+1} - q_n) \right) \tag{2}$$

where $V_{n+1/2}(q)$ is an arbitrary (generally non-linear) interparticle interaction. Note that the potential, $V_{n+1/2}$, depends only on the differences between two adjacent sites; in particular, there is *no* "on-site" potential, $U_{OS}(q_n)$, that depends on the individual coordinates. The (finite) system is considered to be defined on a system of length $L = Na$ with periodic boundary conditions $(q_L, p_L) \equiv (q_0, p_0)$, where actual particle positions are $x_n = na + q_n$. In our analysis the masses $m_n$, as well as interparticle potentials $V_{n+1/2}(q)$, can have *arbitrary dependence on the sites* $n$, though the examples studied in literature to date have mostly had uniform potentials $V_{n+1/2}(q) = V(q)$ and uniform, $m_n = m$, or dimerized $m_{2n} = m_1, m_{2n+1} = m_2$, masses. We require only that the Hamiltonian (2) be invariant under translations $q_n \to q_n + b$ for *arbitrary b*. This requires $U_{OS}(q_n) = 0$ [15].

Our aim is to estimate $\kappa$, the coefficient of thermal conductivity, which is given by the Kubo formula [20]

$$\kappa = \lim_{T \to \infty} \lim_{L \to \infty} \frac{\beta}{L} \int dt g_T(t) \langle J(t) J \rangle_\beta. \tag{3}$$

Here we have written the canonical average of an observable $A$ at inverse temperature $\beta$ as $\langle A \rangle_\beta = \int \Pi_n dp_n dq_n A \exp(-\beta H) / \int \Pi_n dp_n dq_n \exp(-\beta H)$. The order of limits in Eqn (3) is crucial to the precise definition of $\kappa$. In Eqn (3), $J = \sum_{n=0}^{L-1} j_n$ is the total heat current, and $j_n$ is the heat current density [15], given by

$$j_n = \{h_{n+1/2}, h_{n-1/2}\} = \tag{4}$$
$$= \frac{p_n}{2m_n} \left( V'_{n+1/2}(x_{n+1} - x_n) + V'_{n-1/2}(x_n - x_{n-1}) \right).$$

Writing the total Hamiltonian as $H = \sum_{n=0}^{L-1} h_{n+1/2}$, where $h_{n+1/2}$ is the Hamiltonian density

$$h_{n+1/2} = \frac{p_{n+1}^2}{4m_{n+1}} + \frac{p_n^2}{4m_n} + V_{n+1/2}(q_{n+1} - q_n), \tag{5}$$

we find that current density given by (4) satisfies the continuity equation

$$\dot{h}_{n+1/2} = \{H, h_{n+1/2}\} = j_{n+1} - j_n. \tag{6}$$

Here $\{.\}$ is the usual canonical Poisson bracket.

Our approach will be similar to that used by Mazur [21], with a crucial difference: we will average correlation functions over a *finite* rather than *infinite* time domain, $T$. We start with an elementary inequality. For an arbitrary observable $X(t) = X(\{q_n(t), p_n(t)\})$, we have

$$\int_{-\infty}^{\infty} dt g_T(t) \langle X(t) X \rangle_\beta \geq 0 \tag{7}$$

where $g_T(t)$ is a suitable $L^2(R)$ *window* function of effective width $T$, which has the following properties:

(i) $\int_{-\infty}^{\infty} dt g_T(t) = T$.
(ii) $\int_{-\infty}^{\infty} dt g_T^2(t) = T$.
(iii) $\tilde{g}(\omega) := \int_{-\infty}^{\infty} dt g_T(t) e^{i\omega t} > 0$ for all $\omega$.

The natural choice satisfying these conditions is a Gaussian, $g_T(t) = \sqrt{2}\exp(-2\pi(t/T)^2)$. Using elementary Fourier analysis, the above inequality (7) is easily proved by rewriting it as

$$\int d\omega \tilde{g}_T(\omega)\langle S_X(\omega)\rangle_\beta \geq 0 \tag{8}$$

where $S_X(\omega) = \lim_{T\to\infty}\frac{1}{T}\left|\int_0^T dt e^{i\omega t}X(t)\right|^2$ is the power spectrum of the signal $X(t)$. Obviously, $S_X(\omega) > 0$, and given (iii), the inequality (7,8) is clearly fulfilled. We now write the observable $X$ as $X = A + \alpha B$, $\alpha \in R$. Optimizing with respect to the parameter $\alpha$, we arrive at the Schwartz-like inequality

$$\left(\int dt g_T(t)\langle A(t)A\rangle_\beta\right)\left(\int dt g_T(t)\langle B(t)B\rangle_\beta\right) \geq$$
$$\geq \left(\int dt g_T(t)\langle B(t)A\rangle_\beta\right)^2. \tag{9}$$

The above inequality is of quite general use, and we implement it by taking $A \equiv J$ and $B \equiv P$, where $P = \sum_{n=0}^{L-1} p_n$ is the total momentum. For Hamiltonians of the form (2), $P$ is an integral of motion $\dot{P} = \{H, P\} \equiv 0$ due to translational symmetry. Since $P(t) = P$, the above inequality now reads

$$\int dt g_T(t)\langle J(t)J\rangle_\beta \geq T\frac{\langle JP\rangle_\beta^2}{\langle P^2\rangle_\beta}. \tag{10}$$

The rhs of Eqn. (10) can be easily evaluated: $\langle P^2\rangle_\beta = L/\beta$, and $\langle JP\rangle_\beta = \beta^{-1}\sum_{n=0}^{L-1}\langle V'(q_{n+1} - q_n)\rangle_\beta$ since $\langle A(\{q_n\})B(\{p_n\})\rangle_\beta = \langle A(\{q_n\})\rangle_\beta\langle B(\{q_n\})\rangle_\beta$. $\langle V'(q_{n+1} - q_n)\rangle_\beta$ is an average *force* between particles $n$ and $n+1$, i.e. *the thermodynamic pressure* and should not depend on $n$. The pressure can be rewritten through the usual thermodynamic definition

$$\phi \equiv \frac{\partial F}{\partial(La)} = \frac{1}{L}\sum_{n=0}^{L-1}\langle V'_{n+1/2}(x_{n+1} - x_n + a)\rangle_\beta,$$

where $\exp(-\beta F) = \int \Pi_n dp_n dq_n \exp(-\beta H)$. Inserting the above and multiplying with $\beta/L$, we find that the inequality reads

$$\frac{\beta}{L}\int dt g_T(t)\langle J(t)J\rangle_\beta \geq T\phi^2. \tag{11}$$

By implementing the two limits as indicated in (3) we have proved our main result:

**Theorem:** In momentum conserving systems, if the pressure is non-vanishing in the thermodynamic limit $(\lim_{L\to\infty}\phi > 0)$, then the thermal conductivity diverges and $\kappa \to \infty$.

Therefore, we find anomalous energy transport as a simple consequence of the total momentum conservation. The only case in which the pressure is expected to vanish at *any temperature* is when the forces between particles at zero temperature equilibrium are zero $V'_{n+1/2}(0) = 0$, and the interparticle potentials are all even functions $V_{n+1/2}(q) = V_{n+1/2}(-q)$. This is the case for the FPU "$\beta$" problem, where $V_{n+1/2}(q) = \frac{1}{2}q^2 + \beta q^4$ [12, 18, 19], and there the integrated correlation function vanishes for more subtle (dynamical) reasons.

Even if the zero temperature equilibrium forces vanish $V'_{n+1/2}(0) = 0$, we still have non-vanishing finite temperature pressure (due to 'thermal expansion' of a system confined to a fixed volume $La$) whenever interparticle potentials are not even. This is the case for the FPU "$\alpha$" model, $V_{n+1/2}(q) = \frac{1}{2}q^2 + \alpha q^3$, for the modified diatomic Toda lattice [14], $V_{n+1/2}(q) = \exp(-q) + q$, and for the diatomic hard-point 1D gas [22, 14] $V_{n+1/2}(q) = \{0$ if $q > -a; = \infty$ if $q \leq -a\}$. For the usual diatomic Toda lattice [14], $V_{n+1/2} = \exp(-q)$ the pressure is non-vanishing even at zero temperature, since $V'_{n+1/2}(0) \neq 0$.

Given that momentum conservation implies anomalous conductivity, it is natural to ask whether the converse is true: namely, does anomalous conductivity imply that the model conserves momentum ? Two counterexamples show that this result is *not* true. show. First, if one considers a *linear* chain of *optical* phonons—so $V_{n+1/2} \sim (q_{n+1} - q_n)^2$

and $U_{OS} \sim q_n^2$—one can show [23] by a straightforward extension of the arguments of Ref [9] that this momentum non-conserving model nonetheless has anomalous transport. Similarly, there is a momentum *non-conserving* but *integrable* model due to Izergin and Korepin [24] that also shows anomalous conductivity [23]. Finally, let us to stress that in 1D lattices the nature of dynamics, whether it be completely integrable, completely chaotic, or mixed, does not affect our result: if total momentum is conserved and the canonical average of the pressure does not vanish, the transport is anomalous. We shall address the central issue of the necessary and sufficient conditions for normal transport in a forthcoming paper [23].

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